SUPPLEMENTARY MATERIAL

AZT

Thymidine

(Fig. 1-Sup). Differences between the conformer C1 of AZT and dT: (a) in the bond lengths, (b) in the NBO atomic charges.
(Fig. 2-Sup). Relative energies of all the optimum stable conformers in AZT according to the values of the five exocyclic torsional angles: $\chi$, $\beta$, $\gamma$, $\phi$, and $\delta$. 
Distribution of all the optimum conformers according to the values of the exocyclic torsional angles $\phi$, $\gamma$ and $\chi$ versus $\beta$. The stability areas of the conformers are marked in yellow colour.

(Fig. 3-Sup)
(Fig. 4-Sup). Distribution of all the conformers according to the values of the exocyclic torsional angles $\chi$ and $\phi$ versus $v_{\text{max}}$.

(Fig. 5-Sup). An inadequate orientation of the ATP-dT interaction doesn’t lead to a rotation of H5'.

(M052X) -3627.4068251